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Exciton-polariton band structure in quantum-dot lattices

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Abstract. We develop a theory of exciton polaritons in three-dimensional quantum-dot lattices with the period comparable to the light wavelength. A system of the Maxwell equations and nonlocal material relation are used to derive the dispersion equation in a rather general and well-converging form. A possibility of analytical description of the dispersion is questioned and discussed. The photon band structure is calculated for a face-centered-cubic lattice with spherical dots of the radius exceeding the bulk-exciton Bohr radius. The dispersion along the $\Gamma - X$ and $\Gamma - L$ lines is characterized by a strong anticrossing between bare transverse photon and exciton branches and by remarkable overlapping band gaps. Approaching the U and W points the exciton-polariton branches converge and the gap becomes negligible.

Recently van Coevorden et al. [1] have calculated the optical band structure of a three-dimensional (3D) lattice of resonant two-level atoms. They have solved numerically the dispersion equation for light waves in a face-centered-cubic atomic lattice and demonstrated that, in the certain range of parameters, there exists an overlap of photonic band gaps in all directions in the frequency region near the two-level resonance. Here we consider the photonic (or more precisely, exciton-polaritonic) band structure of lattices formed by a 3D periodic array of quantum dots (QDs).

We start from the Maxwell equations

$$\begin{aligned} &\Delta\mathbf{E} - grad\ div\ \mathbf{E} = -\left(\frac{\omega}{c}\right)^2 \mathbf{D}\ , \\ &div\ \mathbf{D} = 0 \end{aligned} \tag{1}$$

for the electric field $\mathbf{E}$ and the displacement vector $\mathbf{D}$. The nonlocal material equation relating $\mathbf{D}$ and $\mathbf{E}$ is taken in the form (see [2])

$$\mathbf{D}(\mathbf{r}) = \varepsilon_b \mathbf{E}(\mathbf{r}) + 4\pi \mathbf{P}_{exc}(\mathbf{r})\ , \tag{2}$$

$$4\pi \mathbf{P}_{exc}(\mathbf{r}) = T(\omega) \sum_{\mathbf{a}} \Phi_{\mathbf{a}}(\mathbf{r}) \int \Phi_{\mathbf{a}}(\mathbf{r}')\mathbf{E}(\mathbf{r}')d\mathbf{r}'\ . \tag{3}$$

Here $\mathbf{a}$ are the lattice translation vectors enumerating quantum dots, $\Phi_{\mathbf{a}}(\mathbf{r}) = \Phi_0(\mathbf{r} - \mathbf{a})$ is the envelope function $\Psi_{exc}(\mathbf{r}_e, \mathbf{r}_h; \mathbf{a})$ of an exciton excited in the $\mathbf{a}$th QD at coinciding electron and hole coordinates: $\Phi_{\mathbf{a}}(\mathbf{r}) = \Psi_{exc}(\mathbf{r}, \mathbf{r}; \mathbf{a})$. The other notations are

$$T(\omega) = 2\pi \frac{\varepsilon_b \omega_{LT} \omega_0 a_B^3}{\omega_0^2 - \omega^2}\ , \tag{4}$$

ω_{LT} and a_B are the exciton longitudinal-transverse splitting and Bohr radius in the corresponding bulk semiconductor, ω_0 is the QD-exciton resonance frequency, ε_b is the background dielectric constant which is assumed to coincide with the dielectric constant of the barrier material. In the following we neglect the overlap of exciton envelope functions $\Psi_{\mathbf{a}}$ and $\Psi_{\mathbf{a}'}$ with $\mathbf{a} \neq \mathbf{a}'$ so that excitons excited in different dots are assumed to be coupled only via electromagnetic field.

It follows from Eq. (2) that $div\ \mathbf{E} = -(4\pi/\varepsilon_b)\ div\ \mathbf{P}_{exc}$ which allows to rewrite the first Eq. (1) as

$$\Delta\mathbf{E} + k^2\mathbf{E} = -4\pi k_0^2 \left(1 + k^{-2} grad\ div\ \right)\mathbf{P}_{exc}\ , \tag{5}$$

where $k_0 = \omega/c$, $k = k_0 n_b = \omega n_b/c$ and $n_b = \sqrt{\varepsilon_b}$.

We seek for Bloch-like solutions of Eq. (5) satisfying the translational symmetry $\mathbf{E}_{\mathbf{K}}(\mathbf{r} + \mathbf{a}) = \exp(i\mathbf{K}\mathbf{a})\,\mathbf{E}_{\mathbf{K}}(\mathbf{r})$ where the wave vector $\mathbf{K}$ is defined within the first Brillouin zone. The exciton-polariton dispersion $\omega(\mathbf{K})$ can be shown to satisfy the equation

$$\mathrm{Det}||\delta_{\alpha\beta} - R_{\alpha\beta}(\omega, \mathbf{K})|| = 0\ , \tag{6}$$

where $\alpha, \beta = x, y, z$, $\delta_{\alpha,\beta}$ is the Kronecker symbol and, for QD lattices,

$$R_{\alpha\beta} = \frac{k_0^2 T(\omega)}{v_0} \sum_{\mathbf{b}} \frac{|I_{\mathbf{K}+\mathbf{b}}|^2 S_{\alpha\beta}(\mathbf{K}+\mathbf{b})}{|\mathbf{K}+\mathbf{b}|^2 - k^2}\ , \tag{7}$$

$$I_{\mathbf{Q}} = \int \Phi_0(\mathbf{r}) e^{i\mathbf{Q}\mathbf{r}} d\mathbf{r}\ ,\ S_{\alpha\beta} = \delta_{\alpha\beta} - \frac{Q_\alpha Q_\beta}{k^2}\ , \tag{8}$$

$\mathbf{b}$ are the reciprocal lattice vectors and v_0 is the volume of the lattice primitive cell.

Similarly to [1] we consider a face-centered-cubic lattice with the lattice constant a and the unit-cell volume $v_0 = a^3/4$. It is convenient to introduce a dimensionless parameter $P = (\pi\sqrt{3}c/a\omega_0 n_b)^3$ and the dimensionless frequency $\Omega = \omega/\omega_0$. The calculation is performed for spherical QDs with the radius R exceeding the Bohr radius a_B in which case we have

$$I_{\mathbf{Q}} = \pi \left(\frac{2R}{a_B}\right)^{3/2} \frac{\sin QR}{QR[\pi^2 - (QR)^2]}\ . \tag{9}$$

Then Eq. (7) can be transformed into

$$R_{\alpha\beta}(\Omega, \mathbf{K}) = N \frac{\Omega^2}{\Omega^2 - 1} \sigma_{\alpha\beta}(\Omega, \mathbf{K})\ , \tag{10}$$

$$\sigma_{\alpha\beta}(\Omega, \mathbf{K}) = \sum_{\mathbf{b}} \frac{f(|\mathbf{K}+\mathbf{b}|R)\, S_{\alpha\beta}(\mathbf{K}+\mathbf{b})}{\Omega^2 - \Omega^2(\mathbf{K}+\mathbf{b})}\ , \tag{11}$$

$$N = \frac{64}{\pi} \frac{\omega_{LT}}{\omega_0} \left(\frac{R}{a}\right)^3\ ,\ f(x) = \left[\frac{\pi^2 \sin x}{x(\pi^2 - x^2)}\right]^2\ , \tag{12}$$

$\Omega(\mathbf{Q}) = cQ/\omega_0 n_b$. Eq. (6) is equivalent to the three separate equations $R_j(\Omega, \mathbf{K}) = 1$ where R_j $(j = 1, 2, 3)$ are eigenvalues of the matrix $R_{\alpha\beta}$. For high-symmetry points of the Brillouin zone, the symmetry imposes certain relations between the $R_{\alpha\beta}$ components

Table 1. Dispersion equations written in terms of $R_{\alpha\beta}$ for different **K** points in the Brillouin zone.

K $(2\pi/a)$	Nonzero components of $R_{\alpha\beta}$	Dispersion equations
Γ (0, 0, 0)	R_{xx}=R_{yy}=R_{zz}	R_{xx}=1
X (0, 0, 1)	R_{xx}=R_{yy}, R_{zz}	R_{xx}=1, R_{zz}=1
L (1/2, 1/2, 1/2)	$R_{\alpha\alpha}$=R_{xx}, $R_{\alpha\beta}$=R_{xy}($\alpha \neq \beta$)	$R_{xx} - R_{xy}$=1, R_{xx}+2R_{xy}=1
W (1/2, 0, 1)	R_{xx}, R_{yy}=R_{zz}	R_{xx}=1, R_{yy}=1
K (3/4, 0, 3/4)	R_{xx}=R_{zz}, R_{yy} , R_{xz}=R_{zx}	$R_{xx}\pm R_{xz}$=1, R_{yy}=1
U (1/4, 1/4, 1)	R_{xx}=R_{yy}, R_{zz}, R_{xy}=R_{yx}	$R_{xx}\pm R_{xy}$=1, R_{zz}=1

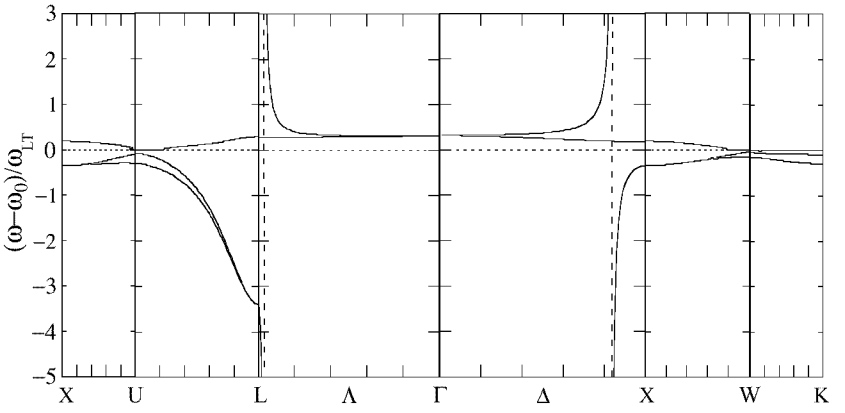

Fig 1. Exciton-polariton dispersion near the exciton resonance frequency ω_0 in a face-centered-cubic lattice of spherical QDs characterized by the following set of parameters: $P = 1.1$, $R/a = 1/4$ and $\omega_{LT}/\omega_0 = 5\times10^{-4}$. The dashed lines show the photon dispersion in the empty lattice, i.e. for $\omega_{LT} = 0$, the dotted horizontal line indicates the value $\omega = \omega_0$.

and the eigenvalues R_j can be readily expressed via these components as illustrated in Table 1 for the points Γ, X, L, W, K and U.

Further simplifications follow taking into account a small value of the parameter N in Eq. (10) since, in semiconductors, the ratio ω_{LT}/ω_0 typically lies between 10^{-4} and 10^{-3}. Then in the frequency region given by the condition $|\Omega - 1| \ll P^{1/3} - 1$ one can readily use the approximate equation $\Omega - 1 \approx (N/2)\sigma_j(1, \mathbf{K})$ where σ_j are eigenvalues of the $\sigma_{\alpha\beta}$ matrix.

Fig. 1 shows the photonic band structure calculated for the dots of radius $R = a/4$ and for $P = 1.1$, $\omega_{LT}/\omega_0 = 5 \times 10^{-4}$. The dispersion on the Λ line is characterized by a giant anticrossing between the branches of bare transverse photon and exciton modes. At the X point, the gap is determined by the separation between the longitudinal and lower transverse branches, it is still remarkable and exceeds $0.5\omega_{LT}$. However near the points U and W the excitron-polariton branches converge and the gap almost disappears. Note that the anticrossing can be described with a high accuracy by retaining in the sum over **b** in Eq. (11) the two terms due to $\mathbf{b} = 0, -(4\pi/a)(0, 0, 1)$ for the Δ points and $\mathbf{b} = 0, -(2\pi/a)(1, 1, 1)$ for the Λ points.

The 3D QD arrays with periods comparable with the light wavelength ($P \approx 1$)

and with sizes exceeding the bulk-exciton Bohr radius could be grown artificially or by embedding semiconductor microcrystals into the pores of porous materials like the synthetic opal [3]. It should be mentioned that the developed theory takes into account a contribution of only one exciton resonance which is valid if the separation between the exciton size-quantization levels is much larger than the bulk value of the exciton longitudinal-transverse splitting, ω_{LT}. In the opposite limit of extremely large bulk-exciton translational effective mass one can use the local material relation $\mathbf{D}(\mathbf{r}) = \varepsilon(\mathbf{r}, \omega)\mathbf{E}(\mathbf{r})$ as it was done by Sigalas et al. [4] for phonon-polaritons in a two-dimensional lattice consisting of semiconductor cylinders.

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